AERONAUTICAL SYSTEMS CENTER
MAJOR SHARED RESOURCE CENTER

COMPAQ SC-45
USER'S GUIDE

September 28, 2005

Release Notes

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Corrected spelling errors. Arranged Released noted in reverse chronological order, so newest updates are near the top.

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Removed references to the -lelan3 compile string, which is no longer needed.

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Corrected miscellaneous errors, updated MPI information.

Issued April 19, 2002.
Preliminary release of User's Guide.

Release Notes

Table of Contents

1. Introduction

This document provides an overview and introduction to using the COMPAQ SC-45 systems, located at the Aeronautical Systems Center (ASC) Major Shared Resource Center (MSRC). The ASC MSRC is located at Wright-Patterson Air Force Base, near Dayton, Ohio. This guide is intended to provide information so that customers who are familiar with the UNIX operating system can create and run their own programs, as well as use existing application software on the COMPAQ SC-45 systems.

1.1 Assumed Background of the Reader

It is assumed that the reader of this guide has a firm grasp of the concepts required to use the UNIX operating system and to program in either the C, C++, FORTRAN 77, FORTRAN 90, or FORTRAN 95 languages. It is also assumed that the reader has read the *ASC MSRC User's Guide*, which contains site specific information about the ASC MSRC. The *ASC MSRC User's Guide* is available from the ASC MSRC Service Center at 1-888-MSRC-ASC (1-888-677-2272), (937)255-0194, or DSN 785-0194. It is also available in postscript and pdf formats as described below in Section 1.7. UNIX training is periodically offered by the ASC MSRC.

1.2 Hardware Overview

The COMPAQ SC-45 systems is a SMP system with 4 CPUs per node. Each CPU is a 1 GigaHertz (GHz) EV6.8 Alpha processor and has a 64 KB primary data cache, a 64 KB primary instruction cache, and 8 MB on-board cache.

1.3 Accessing the COMPAQ SC-40/45

The COMPAQ SC-45 has a total of 836 CPUs, divided into 2 systems (*hpc09* has has 128 nodes, totaling 512 processors and *hpc10* has 81 nodes, totaling 324 processors), with 4 CPUs per node. The fully qualified hostnames of the interactive systems are *hpc09.asc.hpc.mil* and *hpc10.asc.hpc.mil*.

Users are only allowed to login onto the interactive nodes. The other systems are for batch jobs only. Users submit their jobs on *hpc05*, *hpc09* or *hpc10* and the batch system will automatically start their jobs on the other systems based on the load of the system. See the *ASC MSRC User's Guide* for instructions on accessing the machines.

1.4 ASC MSRC Connectivity

Since the COMPAQ SC-45 is an integrated component of the ASC MSRC, user files are Network File System (NFS) mounted from the ASC MSRC High Availability File Server (HAFS) system to the COMPAQ SC-45. When users log into a system, their home ($HOME) directory (which will be the current directory immediately after logging in) physically resides on the file server, but appears to be on the COMPAQ SC-45. The ASC MSRC also supplies archival storage and visualization capabilities.

1.5 ASC MSRC Startup Files

All users are provided a `.cshrc` and `.login` file in their home directory. These files reference standard setup files, maintained by the site administrators in a central location, which set up a standard environment for all MSRC users. These files **should not** be modified.

To set up specific information for your COMPAQ SC-45 session, such as environment variables, path information, terminal information, or command aliases, place them into files called `.personal.cshrc` and `.personal.login`. The standard startup files check your home directory for the existence of these files and executes them if found. Commands related to aliases, prompts, and some environment variables should go into `.personal.cshrc`, while commands related to the type of terminal you are using should go into `.personal.login`. See Section 3 of this guide for more details on the COMPAQ SC-45 computing environment and the *ASC MSRC User's Guide* for more details on startup files.

1.6 The Archive Command

The ***archive*** command is a recently added tool to the ASC MSRC to help users with transferring files to and from $ARC. The basic syntax for the archive command is:

archive get [getopts] file1 [file2 ...]
archive put [putopts] file1 [file2 ...]

More information on the ***archive*** command can be found online via the archive man page (***man archive***).

1.7 Additional Information

Much of the information presented in this document is available online through the man pages and is accessible by typing:

man {command name}

when logged into any COMPAQ SC-45 interactive node.

The *ASC MSRC User's Guide* and this document are all available in pdf and postscript format. They may be downloaded via the ASC MSRC website at

`http://www.asc.hpc.mil/customer/userdocs.`

2. ASC MSRC COMPAQ SC-45

This section details the hardware and software available on the COMPAQ SC-45 and how they are currently configured.

2.1 Hardware

The COMPAQ SC-45 has a total of 836 CPUs. Each CPU is a 1 GHz EV6.8 Alpha processor with a peak speed of 2 GFLOPs, providing a total capacity of approximately 1.67 TFLOPs. Each CPU has a primary data cache of 64 KB, a primary instruction cache of 64 KB, and an on-board cache of 8 MB. At this time, the SC-45 is divided into two separate systems with 128 nodes on one system and 81 nodes on the other. The COMPAQ SC-45 has a SMP architecture with 4 CPUs and 4 GB memory per node.

2.2 COMPAQ SC-45 File System Overview

Diskspace is subdivided into two areas:

- System space (i.e., `/usr`, `/opt`.)
- `/workspace`

2.2.1 COMPAQ SC-45 `/workspace`

`/workspace` is a filesystem local to each machine that users are required to run their jobs in.

I/O on the `/workspace` filesystems is quicker than I/O on a file system mounted from the network (such as your MSRC home directory or archive directory). `/workspace` is intended for the **temporary** storage of data files needed for your application. This includes (but is not limited to) grid files, restart files, input files, and output files. `/workspace` is to be used rather than the `/tmp` and `/usr/tmp` directory areas.

Each user is given a directory named `/workspace/username` where `username` is the user's login name. This directory is created for the user at login via the global `.cshrc` file, if necessary. The global `.cshrc` file also creates the environment variable `$WRK` which is set to `/workspace/username`. The user may use this environment variable as needed.

Workspace on the SC-45's workspace totals 8 TB (4 TB per system) and uses a Parallel File System (PFS) to manage `/workspace.` All nodes have access to `/workspace.`

NOTE: `/workspace` on *hpc09* and *hpc10* are not joined. To view the contents of these workspaces, you will have to login to the appropriate machine to view its workspace.

There is no quota on the amount of disk space a user may use in `/workspace,` but a file scrubber is used to automatically remove old files from `/workspace` to prevent it from becoming filled. The current policy for removing files is on the ASC MSRC web page at

http://www.asc.hpc.mil/overall/policy_procedure/policies/wrkspace_pol.php

This policy is subject to change based on periodic reviews.

The `/workspace` file system is NOT backed up. In the event of deletion or catastrophic media failure, files and data structures are lost. It is the user's responsibility to transfer files that need to be saved to a location that allows permanent storage. Two possibile locations are the user's $HOME directory space on the file server or the user's $ARC directory on the archival storage system.

2.3 COMPAQ SC-45 Tru64 UNIX Operating System

The COMPAQ SC-45 runs Tru64 UNIX, a 64-bit, multiuser/multitasking operating system based on components from Berkeley Software Distribution (BSD) versions 4.3 and 4.4 and AT&T UNIX System V, Release 4.0.

2.4 Available Software

Software currently available on the COMPAQ SC-45 includes the Digital FORTRAN 77, FORTRAN 90, FORTRAN 95, C, and C++ compilers; Elan MPI and many third party software packages. A complete list of software is maintained on the ASC MSRC web page (http://www.asc.hpc.mil/software/).

2.5 Development

The COMPAQ SC-45 has several tools available to help develop, compile, and analyze programs.

The compilers on the COMPAQ SC-45 are optimizing and parallelizing compilers that can generate 64-bit and 32-bit code. The FORTRAN 90 compiler also supports High Performance Fortran (HPF) directives.

The COMPAQ SC-45 has the Digital Extended Math Library (DXML). This is a collection of mathematical and scientific libraries including Basic Linear Algebra Subprograms (BLAS) levels 1, 2, and 3; LAPACK; Fast Fourier Transforms (FFTs); and convolutions.

The Ladebug debugger on the COMPAQ SC-45 is a fully symbolic debugger with a graphical user interface. This debugger offers the following features:

- perform source-level debugging
- attach to running process
- debug programs with shared libraries
- debug multithreaded applications
- debug multiprocessor applications, including programs that fork/exec

Documentation for these compilers, libraries, and tools is available online in the man page by executing a man on `f95` (the `f95` man page covers `f77`, `f90` and `f95`), `cc`, `cxx`, `dxml` and `ladebug`.

3. Program Development

Program development in the COMPAQ SC-45 computing environment is similar to that used in a typical UNIX environment. However, the user must take additional steps to utilize the multiple processors available.

3.1 Parallel Processing

Users may utilize multiple CPUs to execute their programs. The compilers are capable of creating parallel programs through the use of compiler directives and parllel standards such as Message Passing Interface (MPI) and OpenMP.

3.1.1 MPI

The goal of MPI is to develop a widely used standard for writing message-passing programs. As such the interface attempts to establish a practical, portable, efficient, and flexible standard for message passing.

You can compile MPI programs on the COMPAQ SC-45 using the following command line options.

For MPI and FORTRAN codes:

f77 -lmpi -lelan -o prog prog.f

f90 -lmpi -lelan -o prog prog.f

For MPI and C/C++ codes:

cc -lmpi -lelan -o prog prog.c

cxx -lmpi -lelan -o prog prog.c

Other compiler options are available. Please consult the man pages for the compiler you are using for more information.

To run an MPI program on the COMPAQ SC-45, you must submit it to the Resource Management System (RMS) via the ***prun*** command. The ***prun*** command is discussed in greater detail later in this guide and more information on prun can be obtained by executing a ***man prun*** while logged into the COMPAQ SC-45.

More information on MPI can be obtained from:

`http://www.mpi-forum.org`

3.1.2 OpenMP

OpenMP is a specification for a set of compiler directives, library routines, and environment variables that can be used to specify shared memory parallelism in FORTRAN and C/C++ programs.

Creating an OpenMP program is done through OpenMP directives in the source code and by adding the ***-omp*** flag to your compile string.

To run an OpenMP program, you must first tell the program how many threads (processors) to use. This is achieved through the OMP_NUM_THREADS environment variable. To set this variable, use the following command in ***csh***:

setenv OMP_NUM_THREADS x

where *x* is the number of CPUs you wish to run on.

For more information on OpenMP and its directives, please see the following page:

`http://www.openmp.org`

3.2 FORTRAN Programming

The default FORTRAN compiler on the COMPAQ SC-45 is the Digital FORTRAN compiler. The FORTRAN compiler commands are f77, f90 and f95. These commands utilize the same compiler built with different default options. These optimizing and parallelizing compilers can generate 64-bit and 32-bit code. The Digital FORTRAN 77 compiler is fully compliant with the ANSI X3.9-1978 and FIPS PUB 69-1 standards defined for FORTRAN 77. The Digital FORTRAN 90 fully complies with the ANSI X3.198-1992 and ISO/IEC 1539:1991(E) standards definition for FORTRAN 90.

Compiling a FORTRAN program on the SC-40/45 is similar to compiling a program on a typical UNIX system.

f95 -o prog prog.f

This command creates an executable called `prog`. The program is run by typing the program name at the system prompt.

./prog

Further optimization is available through the use of compiler flags and compiler directives. Please check the `f77`, `f90` and `f95` man pages for more details.

3.3 C/C++ Programming

The DEC C and Digital C++ compilers are available on the COMPAQ SC-45. These compilers are capable of optimizing and parallelizing code. The DEC C compiler fully complies with the ANSI X3.159-1989 and ISO/IEC 9899:1990 standards definition for C. The Digital C++ compiler fully complies with the ISO/IEC 14882:1998 standard definition for C++.

Compiling a C program on the COMPAQ SC-45 is similar to compiling a C program on a typical UNIX system.

cc -o prog prog.c

Compiling a C++ program is also similar to other systems.

cxx -o prog prog.C

These commands will create an executable program in a file called ***prog***. The program is executed by entering

./prog

Further optimization is available through the use of compiler flags and compiler

directives. Please consult the cc or cxx man pages for more details.

3.4 Libraries

3.4.1 Math and Science Libraries

The COMPAQ SC-45 has DXML, a collection of mathematical and scientific libraries including Basic Linear Algebra Subprograms (BLAS) levels 1, 2, and 3; LAPACK, a collection of solvers for dense linear algebra problems, including linear equations, linear least squares problems, eigenvalue problems, and singular value decomposition problems; Fast Fourier Transforms (FFTs); and convolutions. Both single-threaded and multi-threaded routines are available and select routines have been highly optimized to greatly improve performance. Users should use these library routines whenever possible.

This library is not automatically included in the link path. The user must specify the library when linking as in the following examples.

f90 -o prog prog.f -ldxml
cc - o prog prog.c -ldxml

If the user wants to use the parallel version of this library, they must use the following directive:

f77 -o prog prog.f -ldxmlp
cxx -o prog prog.c -ldxmlp

Please consult the `dxml man` page for more details on the routines that are available.

4. Running Jobs on the COMPAQ SC-45

4.1 Interactive Use

Interactive use is allowed, particularly for program development, including debugging and performance improvement, job preparation, job submission, and the preprocessing and postprocessing of data. However, only one node on each of the COMPAQ SC-45 systems is available for interactive use and interactive jobs are limited to 4 CPUs with 15 minutes of CPU time per process. Jobs with larger resource requirements must be submitted to the batch queues.

4.2 Batch Use

The COMPAQ SC-45 uses the Load Sharing Facility (LSF). LSF is a networked subsystems for submitting, monitoring, and controlling a work load of batch jobs on one or more systems. It provides services to monitor queue activity and to delete queued or running jobs. In the event of an orderly system shutdown, LSF jobs will be rerun from the beginning of the job (unless they are specifically marked not to be rerun). More information about LSF is available at

```
http://www.platform.com/products/HPC
```

Currently, jobs can be submitted from any SC-45 interactive node, however, they can run on *hpc09* or *hpc10* once submitted.

4.2.1 Queues Available on the COMPAQ SC-45

The ASC MSRC COMPAQ SC-45 has three user queues: express, default, and background. These queues are available 24 hours a day, 7 days a week.

The Debug queue accepts jobs that require up to 32 CPU, 1 hour of walltime, and 32 GB of memory. This queue is intended for short runs.

The Default queue is available for production work. Jobs that are submitted without any queue specified will go to the default queue. The Default queue is divided into subqueues, but users do not submit jobs directly to these subqueues. Rather, the user specifies the number of CPUs, the CPU time, and memory requirements using the ***bsub*** options listed in Section 4.2.4. The job is then routed to the appropriate subqueue.

The background queue is also available for production work. Jobs run in the background queue are not charged against a user's allocation. However, jobs in the background queue are assigned the lowest priority and are only started when utilization of the machine is low.

The upper limits of job resources for the COMPAQ SC-45 queues are available on the web at

```
http://www.asc.hpc.mil/overall/policy_procedure/policies/
batchqueue.php
```

These limits are subject to change based on periodic review of system utilization and system configuration.

4.2.2 Preparing Jobs

Before a user submits a job, they should prepare a job script. A job script is a

UNIX shell script that contains all the commands the user will execute during the job. LSF will place the error and output files in the directory the job was submitted from, so scripts must be written with this in mind. Here is a sample job script.

```
#
#Change to WORK_DIR directory and copy input file.
#
cd $WORK_DIR
archive get -C {directory in $ARC} {filename}
#
#Run the analysis.
#
{My Program}
#
#Archive output and remove $WORK_DIR
#
tar cvf ../{output filename}.tar .
archive put -C {directory in $ARC} ../{output filename}.tar
rm -rf $WORK_DIR
#
#Exit the script.
#
exit
```

This script copies files from the archival storage system $ARC to the user's $WORK_DIR directory. The $WORK_DIR directory is a directory created by LSF for users to run their batch jobs that maps to `/workspace/username/<LSF jobID>.<submithost>`. For example, if user joe submitted a job from hpc09 and was given an LSF jobID of 12345, his $WORK_DIR variable in LSF would expand to `/workspace/joe/12345.hpc09-0/`

This directory has certain protections from the `/workspace` scrubber, as long as the job is running, plus five days, this directory and the files/subdirectories within it will not be removed.

The script then changes to the $WORK_DIR directory, runs the program, copies two output files to permanent storage (one to the $HOME directory, one to the archival storage system $ARC), and then deletes the remaining files, the $WORK_DIR directory and exits.

NOTE: $WORK_DIR variable only exists in LSF, so you will not be able to change to that directory using the variable $WORK_DIR. To view your $WORK_DIR directory, login to the system your job is running on and change directories to $WRK. If you are logged into the correct system and your job is running, there will be a directory who's name will reflect the JobID of the job you are running. If you have multiple jobs running, you will have a directory for each job running. Note: You will not have a $WORK_DIR for a job that is not in a Run status.

4.2.3 The PRUN Command

Due to the Quadrics Switch, the COMPAQ SC-45 uses Resource Management System (RMS) to control system resources on the compute

nodes. Users interface with RMS via the prun command, however, due to the way LSF communicates to RMS, the PRUN command is only required for MPI jobs. It is not recommended that users use PRUN for SMP jobs on the SC-45.

For SMP or serial jobs, use:

prun -N 1 -c {Number of processors} {my program} > {output.file}

For MPI or Parallel jobs, use:

prun -n {number of CPUs} {my program} > {output.file}

Using PRUN on the COMPAQ SC-45 for *MPI* jobs is a requirement. Jobs not using the PRUN command are in danger of overloading the system and will be killed.

Because of the way LSF interacts with PRUN, you must redirect your output to a separate file such as in the examples above. For more information concerning prun and the Quadrics Switch upgrade, please consult the man pages on PRUN or the ASC MSRC website.
(http://www.asc.hpc.mil/customer/userdocs)

4.2.4 Submitting Jobs

Once a job script is prepared, the `bsub` command is used to submit the script to LSF. The command has the following syntax:

```
bsub < script
```

Some important LSF options used on the COMPAQ SC-45 are as follows (type `man bsub` for a complete list of options available.

-q *queue*	Specifies the name of the queue to which the job will be submitted. For a list of allowable queues, please see: http://www.asc.hpc.mil/overall/policy_procedure/policies/batchqueue.php. *The default queue is `q004`.
-n *n*	Specifies the number of CPUs the job will use. *The default number of CPUs is 1.
-W *hh:mm*	Specifies the time limit for the job in walltime. The time should be specified in the hh:mm format (e.g., 15:00). *This is a required field, there is no default.
-M *n*	Specifies the memory size limits for the job in kilobytes. *The default is 1GB.

-o *outfilename*	Standard output (stdout) for the job is written to *outfilename*. *If you do not specify an output filename, LSF emails the output to your ASC email account.
-e *errfilename*	Standard error (stderr) for the job is written to *errfilename*. The default name is *jobname*.e*nnn* where *nnn* is the LSF identifier. *If you do not specify an error filename, LSF emails the error information to your ASC email account.
-J *jobname*	Specifies the name of the job. *This is a required field, there is no default.
-P *account*	Specifies the account number to charge to. *This is a required field, there is default.
-a [SMP|MPI|MIX]	Specifies how jobs should be spread across nodes, if at all. SMP and MIX forces all CPUs to be allocated on a single node while MPI allows CPUs to be spread across multiple nodes. *This is a required field, there is no default.

When a job is submitted to LSF, a unique identifier is assigned to the job by the batch system similar to below:

```
2079.hpc09-0.asc.hpc.mil
```

This identifier is needed when deleting a job.

Options of `bsub` commands are specified within the script file itself. The options are specified using syntax similar to PBS, but each line that contains an option must begin with the `#BSUB` string. Options that are specified within the script file must precede the first executable shell command of the file as in the following example.

```
#!/bin/csh
#BSUB -q regular
#BSUB -n 1
#BSUB -W 168:00
#BSUB -J test
#BSUB -o test.out
#BSUB -e test.out
#BSUB -a MPI
#BSUB -P WP+WPASC00000000*
```

*This is an example number. To find your account number, check your $ACCOUNT variable using

echo $ACCOUNT

More sample batch scripts can be found at the following URL:

```
http://www.asc.hpc.mil/customer/userdocs/samples/
samplebatch.php
```

4.2.5 Monitoring Jobs

The `bjobs` command is used to report the status of the batch jobs that are currently queued or running. Type `man bjobs` for information about `bjobs` and the options that are available.

The `bjobs` command lists all jobs that are running and queued.

bjobs -u all

```
JOBID   USER     STAT          QUEUE       FROM_HOST    EXEC_HOST   JOBNAME    SUBMIT_TIME
3373    user1    PEND          normal      hpc09-a                  test       Feb 5 15:22
3971    user2    RUN           normal      hpc09-a      hpc09-b     test       Feb 5 15:22
```

Here is an explanation of the fields in the `bjobs` output.

Table 1: Fields from `bjobs`

Item	Meaning
JOBID	A unique identifier that consists of the original request number and the machine from which the request was submitted. Format is *nnn*, where *nnn* is an integer.
USER	Username of person submitting the job.
STAT	Job status. “RUN” indicates the job is running; “PEND” indicates the job is queued.
QUEUE	Name of the queue where the job is waiting or executing.
FROM_HOST	Cluster domain from where the job was submitted from.
EXEC_HOST	Cluster domain where the job is running.
JOBNAME	Name of the job. This is either the name of the script file submitted to LSF or the name chosen with the -J flag.
SUBMIT_TIME	The date and time the jobs was submitted on.

4.2.6 Deleting Jobs

In LSF, queued or running jobs are removed using the `bkill` command. The syntax is

bkill *request-id*

where *request-id* is the LSF identifier number.

Example:

bjobs

```
JOBID   USER     STAT          QUEUE       FROM_HOST    EXEC_HOST   JOBNAME    SUBMIT_TIME
3373    user     PEND          normal      hpc10-a      hpc10-b     test       Feb 5 15:22
```

bkill 3373

5. Customer Service

5.1 Customer Service Center

For customer assistance, call the ASC MSRC Service Center at 1-888-MSRC-ASC (1-888-677-2272), (937)255-0194, or DSN 785-0194, or send e-mail with a description of the problem to msrchelp@asc.hpc.mil. The support analysts will help with anything related to ASC MSRC: third party software, UNIX, the different ASC MSRC computers, etc. If you have any questions about the ASC MSRC, contact the Service Center first. If your problem or question is beyond the scope of their expertise, they will refer you to the appropriate resource.

5.2 ASC MSRC Support

In-depth technical inquiries and problems are forwarded to the ASC MSRC Customer Assistance and Technology Center (CATC), which pursues such inquiries and problems through resolution as rapidly as possible. The ASC MSRC CATC will attempt to determine the nature of the problem, then identify and coordinate whatever resources are needed to resolve the problem.

The ASC MSRC also offers training classes, which provide an introduction to UNIX and the ASC MSRC. Intermediate and advanced classes on selected topics are also periodically announced on the Programming Environment and Training (PET) section of the ASC MSRC homepage. Topics for such classes may be requested through the Customer Service Center.

The ASC MSRC CATC is ready to support in an advisory capacity any engineer or scientist who is (or potentially is) an ASC MSRC user.

5.3 ASC MSRC Website

The ASC MSRC website is the best source for current ASC MSRC information. To access the ASC MSRC website simply access this URL: http://www.asc.hpc.mil.

Some of the topics found on the website include:

APPLICATIONS
Short and long descriptions of current ASC MSRC applications

`http://www.asc.hpc.mil/software/`

SYSTEMS
Information on ASC MSRC servers and Archival Storage

`http://www.asc.hpc.mil/hardware/`

CUSTOMER SERVICE
Available Customer Services

`http://www.asc.hpc.mil/customer/`

ONLINE DOCUMENTATION
Listings of the ASC MSRC User Guides are available for viewing. Instructions are given on obtaining postscript versions.

`http://www.asc.hpc.mil/customer/userdocs/`

VISUALIZATION LAB INFORMATION

Current status and other information about the Visualization Lab.

`http://www.asc.hpc.mil/sciviz/`

TRAINING

Current course offerings and schedule

`https://okc.erdc.hpc.mil/wpmjsp/class_listing.jsp`

FREQUENTLY ASKED QUESTIONS

Submit questions and read about various topics (such as “Customizing Your Environment”)

`http://www.asc.hpc.mil/`

POLICIES AND PROCEDURES

The latest policies regarding usage of the ASC MSRC resources.

`http://www.asc.hpc.mil/overall/policy_procedure/`

Appendix A. COMPAQ SC-45 Usage Hints

The following are tips and hints for the effective use of the COMPAQ SC-45.

A.1 Runtime Considerations

A.1.1 Batch use is recommended

The COMPAQ SC-45 system allocates more resources to batch jobs than for interactive use. Users will obtain the best throughput for long running or large memory jobs by submitting jobs to the batch queues.

A.1.2 Request only the time and memory needed

When submitting a job, choose the smallest queue that accommodates the job's time and memory requirements. Jobs that request significantly more resources than are actually needed can result in longer wait times and inefficient use of the machine.

A.1.3 PRUN usage

All MPI jobs on the COMPAQ SC-45 are required to use ***prun***. Jobs that are required to use ***prun*** but do not, are in danger of overloading the system and will be killed without warning.

A.2 Files and Filespace

A.2.1 File Management in `/workspace`

A file scrubber is used to automatically remove old files from `/workspace` to prevent `/workspace` from becoming filled. The policy for removing files from `/workspace` is available on our website. However, users are encouraged to remove files from `/workspace` when they are no longer needed. This will minimize the overhead needed to enforce this policy.

The `/workspace` filesystem is not backed up. It is the user's responsibility to transfer files that need to be saved to a location that allows permanent storage. Two possibilities are the user's $HOME directory space on the file server or the user's $ARC directory on the archival storage system.

A.2.2 Archival Storage

The directories of the ASC MSRC Archival Storage system are NFS mounted on the COMPAQ SC-45. However, copying or moving (i.e., `cp` or `mv`) large files to or from an NFS file system is very slow. `ftp` and `rcp` afford the quickest means to transfer files to and from the archival storage system.

To open an `ftp` session from the COMPAQ SC-45 to the archival storage system, type the following command.

ftp $msas

The `archive` command is more convenient to use than ***ftp*** within a script.

The first example below copies a file from the archive storage system to the local system. The second example copies a file from the local system to the archive storage system.

archive get archive_filename local_filename

archive put local_filename

`archive_filename` and `local_filename` can be the same. For more details about the Archival Storage system, see the *Archival Storage User's Guide*, located at:

`http://www.asc.hpc.mil/customer/userdocs/guides.htm`

A.2.3 Keep I/O local to the system

The `/workspace` filesystems are local to the COMPAQ SC-45 via a RAID 5 storage. Although `$HOME` is NFS-mounted internally to the compute nodes, I/O access from `/workspace` will be faster than from the HAFS.

Here is a sample script that copies two input files (one from the $HOME directory, one from the archival storage system) and a program to the user's `/workspace` directory, changes to the `/workspace` directory, runs the program, copies two output files to permanent storage (one to the $HOME directory, one to the archival storage system), and then deletes the remaining files.

```
cd $WRK
cp $HOME/small.input $WRK
archive get big.input $WRK
archive get prog $WRK
prog
archive put big.output
mv small.output $HOME
rm small.input big.input prog big.output
```

A.3 Helpful COMPAQ SC-45 Websites

A.3.1 COMPAQ

`http://www.COMPAQ.com/`